Contrast Transfer Theory for Transmission Electron Microscopes Equipped with a Wien-Filter Monochromator

M. Lentzen and A. Thust

Ernst Ruska Centre for Microscopy and Spectroscopy with Electrons, Institute of Solid State Research, Research Centre Jülich, 52425 Jülich, Germany

The past two decades have seen major improvements of transmission electron microscopes with respect to the information limit and the interpretable resolution of structure images. The combined use of new instrumentation, such as field-emission sources, more stable lens and high-voltage power supplies, and, eventually, spherical-aberration correctors, provides an interpretable resolution just penetrating the sub-Ångström scale.

Attempts for further improvement are made today by reducing the deleterious influence of the chromatic aberration through the use of gun monochromators. These devices reduce the energy spread of electrons emitted by the source at the cost of brightness. One of the new monochromators, of the Wien-filter type [1], images incoming electrons into an energy dispersive plane, cuts out electrons of a desired small energy interval by means of a slit, and lets the outgoing electrons pass through the high-voltage accelerator and the illumination system to form the illumination cross-over, for example above the specimen under investigation.

The illumination cross-over of a Wien-filter monochromator has a shape much different from that of traditional illumination systems. The linear energy dispersion introduced is still present at the cross-over plane, that is, electrons of different energy appear to impinge from different directions onto a certain point in the object plane. Figure 1 displays a model of the resulting effective source: Electrons with energy E_0 travel straight on, those with energies larger than E_0 are incident from the right, and those with an energy smaller than E_0 are incident from the left. The respective change of the wavevector \mathbf{K} is traced by the wavevector \mathbf{Q} . The vector \mathbf{q} traces an additional direction change, still present for each energy, due to the finite size of the field-emission source.

The traditional imaging model for the contrast transfer under partially coherent illumination [2, 3] is hence no more valid, because it assumes identical illumination disks, spanned by q, for different electron energies. This work was dedicated to a full recalculation of the contrast transfer using the transmission cross-coefficient formalism to describe high-resolution imaging for a microscope equipped with a Wien-filter monochromator, using the illumination model described before.

The most prominent change to the standard high-resolution imaging model [2, 3], which will affect not only future image calculations but also wave function restoration using electron holography or through-focus series reconstruction, has to be made for the damping envelopes describing the effects of partial coherence. The well-known envelopes for spatial and temporal coherence, $E_S(g, h)$ and $E_F(g, h)$, for the two-beam interference of diffracted beams g and h, stay unchanged, but an additional new envelope $E_M(g, h)$ occurs, due to the dispersion of the effective source. The resulting formulae for the first-order expansion are lengthy; therefore we display here, due to limited space, only the envelopes for the linear interferences:

$$E_{s} = \exp\left(-\pi^{2} q_{0}^{2} |\nabla \chi|^{2}\right), \quad E_{F} = \exp\left(-\pi^{2} \Delta_{F}^{2} \left(\frac{\partial \chi}{\partial Z}\right)^{2}\right), \quad E_{M} = \exp\left(-\pi^{2} \Delta_{M}^{2} \left(\frac{\partial Q}{\partial Z} \nabla \chi \cdot \vec{e}_{Q} + \frac{\partial \chi}{\partial Z}\right)^{2}\right),$$

with the aberration-function $\chi(\mathbf{g})$ of the objective lens, the lens defocus Z, the semi-convergence angle of the field-emission source q_0 , the effective defocus spread Δ_F due to high-voltage and lenscurrent instabilities, the effective defocus spread $\Delta_M = C_C \Delta E_M / E_0$ due to the energy spread ΔE_M left over by the monochromator, the constant of the chromatic aberration $C_{\rm C}$, the dispersion of the effective source $\partial Q/\partial Z$, and a unit vector $e_{\rm Q}$ along the dispersion axis.

The simulation of the combined effect of the three envelope functions, displayed in Figure 2, shows a notable effect of the new illumination system: For a spherical-aberration corrected microscope with an information limit of 0.08 nm the contrast transfer becomes asymmetrical for diffraction vectors g and -g upon defocussing the objective lens, here by a moderate value of ± 50 nm. Depending on the amount of defocus high spatial frequencies belonging to one half of the diffraction plane are transmitted poorer. That is, details of the object structure may appear asymmetrical to the operator, and work with such an instrument is restricted to a defocus interval around Gaussian defocus, depending on the strength of the dispersion. The worst of the mentioned effects is, however, the loss of valuable high-resolution information.

References

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- [3] H. Pulvermacher, Optik 60 (1981) 45.



Fig. 1. The effective source for an illumination system equipped with a Wien-filter monochromator. An image of the field-emission source, traced by q, is displaced by a wavevector Q related to an energy change of ΔE . Thus electrons with energy $E_0 + \Delta E$ have an apparent illumination tilt of Q/K.



Fig. 2. The envelope $E_{\rm s}(\mathbf{g}) E_{\rm F}(\mathbf{g}) E_{\rm M}(\mathbf{g})$ of the linear interferences for $E_0 = 300$ keV, defoci -50 nm (left), 0 nm (centre), +50 nm (right), and an information limit of 0.08 nm. The frame coordinates run from -12 nm⁻¹ to +12 nm⁻¹; white denotes a transmission of 1, black a transmission of 0.